# JOURNAL OF MOLECULAR SPECTROSCOPY

## **VOLUME 18, 1965**

Edited by HARALD H. NIELSEN

Associate Editor K. NARAHARI RAO

### Editorial Advisory Board

G. Herzberg

K. K. Innes

Richard C. Lord

P.-O. Löwdin

M. Migeotte

Ian Mills

Robert S. Mulliken

John G. Phillips

John R. Platt

G. B. B. M. Sutherland

H. L. Welsh

E. Bright Wilson, Jr.



Bryce L. Crawford, Jr.

David M. Dennison

H. S. Gutowsky

G. Amat

Børge Bak H. J. Bernstein

# ACADEMIC PRESS

NEW YORK and LONDON

Copyright<sup>©</sup> 1965, by Academic Press Inc.

#### ALL RIGHTS RESERVED

No part of this volume may be reproduced in any form by photostat, microfilm, or any other means, without written permission from the publishers.

#### **CONTENTS OF VOLUME 18**

Number 1, September 1965

HAZIME SAITÔ AND KENKICHI NAKADA. Studies on Oxime Hydrochlorides. Part II. The Paramagnetic Anisotropy Effect of the Hydroxyimino	
Group	1
Monisha Bose, Nemai Das, and Nikhilesh Chatterjee. Nuclear	
Magnetic Resonance of N <sup>14</sup> Bonded to Carbon	32
20 000 to 54 000 cm <sup>-1</sup> .  Philip E. Stevenson. Effects of Chemical Substitution on the Electronic Spectra of Aromatic Compounds. Part IV. A General Theory of Substituent Effects and its Application to the Spectra of the Flower Pig-	42
ments.	51
M. Y. DeWolf. The NMR Spectra of Dimethyl Methyl Phosphonate J. L. Duncan. Limitations of the Urey-Bradley Model in Normal Coor-	59
dinate Analyses	62
HOWARD R. GORDON AND T. K. McCubbin, Jr. The 15-Micron Bands of	
$\mathrm{C^{12}O_2^{16}}$	73
A. Adamson and T. M. Dunn. Spin Forbidden Bands in Cr III Hex-	
amine	83
Donald G. Burkhard and Wesley E. Brittin. The Asymmetric Top—	-
An Analytical Treatment.  T. C. Chiang and R. M. Hammaker. The Carboxyl Proton Chemical	87
Shift of Trimethylacetic Acid Monomers in Carbon Tetrachloride	110
E. A. TRIAILLE AND C. P. COURTOY. Further Evidence for Perturbations	
in the Infrared Spectra of Carbonyl Sulfide	118
Papers Accepted for Publication.	129
Number 2, October 1965	
P. J. Krueger and H. D. Mettee. Spectroscopic Studies of Alcohols. Part VII. Intramolecular Hydrogen Bonds in Ethylene Glycol and	
2-Methoxyethanol	131
D. A. HUTCHINSON AND H. F. HAMEKA. Rotational Intensities of a Mag-	
netic Rotation Spectrum for a Diatomic Molecule	141
J. F. Scott and K. Narahari Rao. Infrared Absorption Bands of Acety-	
lene. Part. II. Effect of Vibrational <i>l</i> -type Doubling	152

Y. DIAMANT, R. M. HEXTER, AND O. SCHNEPP. The Near Ultraviolet Spectra of Benzene in Inert Solid Solutions	158
D. H. RANK, UWE FINK, AND T. A. WIGGINS. High Resolution Measurements on the Infrared Absorption Spectrum of HBr.	170
R. A. Ashby and R. L. Werner. The Vibration-Rotation of HNCO Between 1200-450 cm <sup>-1</sup> .	184
Gary C. Graham and Walter D. Jones. Observation of Delocalization Intensity in the Infrared Bands of the Formate Ion	202
$\nu_3$ Band of $^{15}\mathrm{N}_2{}^{18}\mathrm{O}$ . Note	212
MARTIN J. REISFELD AND LLEWELLYN H. JONES. Raman Spectra of Some Cyanide Complexes of Copper	222
Papers Accepted for Publication	227
Number 3, November 1965	
I. Kovács. On the Triplet Terms of the TiO Molecule	229
Spectrum and Dipole Moment of Azulene  J. T. Bell and R. E. Biggers. The Absorption Spectrum of the Uranyl Ion in Perchlorate Media. Part I. Mathematical Resolution of the Over-	239
lapping Band Structure and Studies of Environmental Effects	247
acetonato Osmium (III). G. H. DIEKE AND S. P. CUNNINGHAM. Bands of D <sub>2</sub> and T <sub>2</sub> Originating	276
from the Lowest Excited <sup>1</sup> $\Sigma_g$ States $(1s\sigma)$ $(2s\sigma)^1$ $\Sigma_g$ and $(2p\sigma)^{21}$ - $\Sigma_g$ Marshall L. Ginter. The Spectrum and Structure of the He <sub>2</sub> Molecule. Part III. Characterization of the Triplet States Associates with the	288
UAO'S 3s and $\mathrm{sp}\pi$ . Richard Nelson and Louis Pierce. Microwave Spectrum, Structure,	321
and Barrier to Internal Rotation of Acetone  Papers Accepted for Publication	
Number 4, December 1965	
Hazime Saitô and Kenkichi Nukada. Studies of Oxime Hydrochlorides Part III, Long Range Anisotropy Effect of Hydroxyimino Groups of Dioximes	955
B. S. Snowden, Jr. and W. H. Eberhardt. Magnetic Rotation Spectrum of Singlet-Triplet Transitions. Part II. Pyrazine.	
UWE FINK, T. A. WIGGINS, AND D. H. RANK. Frequency and Intensity Measurements on the Quadrupole Spectrum of Molecular Hydrogen	384
MICHEL COURTOIS AND LESLIE S. FORSTER. The Emission Spectra of Dilute Crystals of Chromium $\beta$ -Diketone Complexes.	

Sister Noël Dreska; K. Narahari Rao, and L. H. Jones. $\nu_3$ of Boron	
Trifluoride	404
RALPH W. PARSONS AND JAMES A. ROBERTS. The Doppler Contribution	
to Microwave Line Widths	412
D. H. RANK, A. G. St. PIERRE, AND T. A. WIGGINS. Rotational and	
Vibration Constants of CO	418
J. Morris Weinberg, E. S. Fishburne, and K. Narahari Rao. "Hot"	
Band of CO at 4.7 Microns Measured to High J Values	428
Beat Meyer. The Ultraviolet Spectrum of AsO	443
Note	
J. F. Scott and K. Narahari Rao. Reconsideration of Vibrational	
l-Type Doubling in Acetylene	451
Papers Accepted for Publication	453
Author Index	454
Subject Index	455

